Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:38 am BST

PDB ID	:	1Z9H
Title	:	Microsomal prostaglandin E synthase type-2
Authors	:	Yamada, T.; Komoto, J.; Watanabe, K.; Ohmiya, Y.; Takusagawa, F.
Deposited on	:	2005-04-02
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

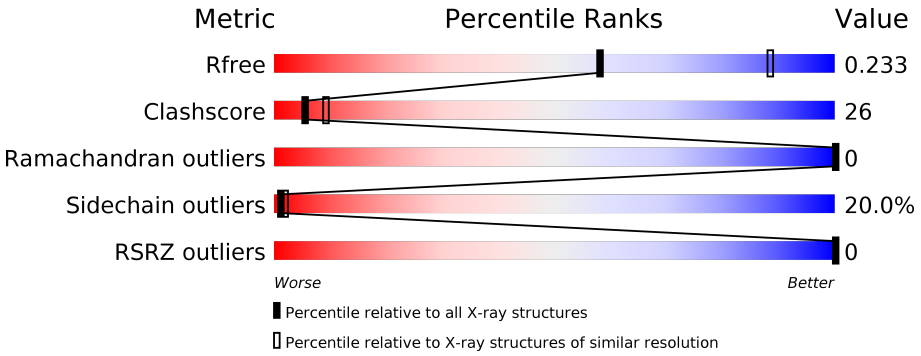
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	290	50% 37% 8% 6%
1	B	290	48% 37% 10% 6%
1	C	290	47% 39% 8% 6%
1	D	290	48% 38% 9% 6%

2 Entry composition

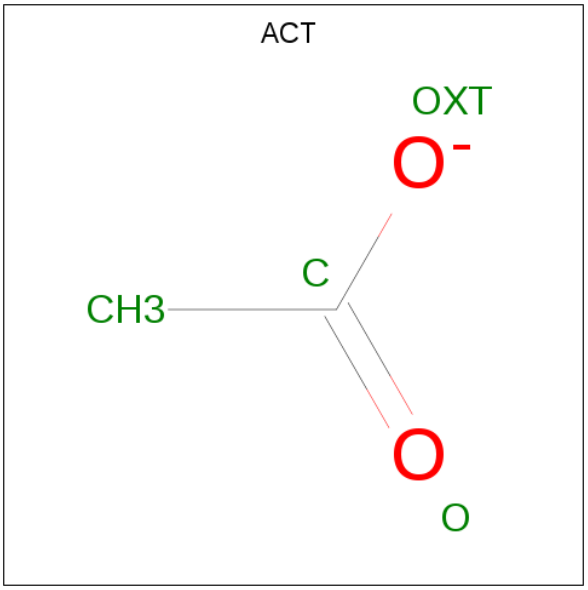
There are 5 unique types of molecules in this entry. The entry contains 9064 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called membrane-associated prostaglandin E synthase-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2214	1421	376	407	10			
1	B	274	Total	C	N	O	S	0	0	0
			2214	1421	376	407	10			
1	C	274	Total	C	N	O	S	0	0	0
			2214	1421	376	407	10			
1	D	274	Total	C	N	O	S	0	0	0
			2214	1421	376	407	10			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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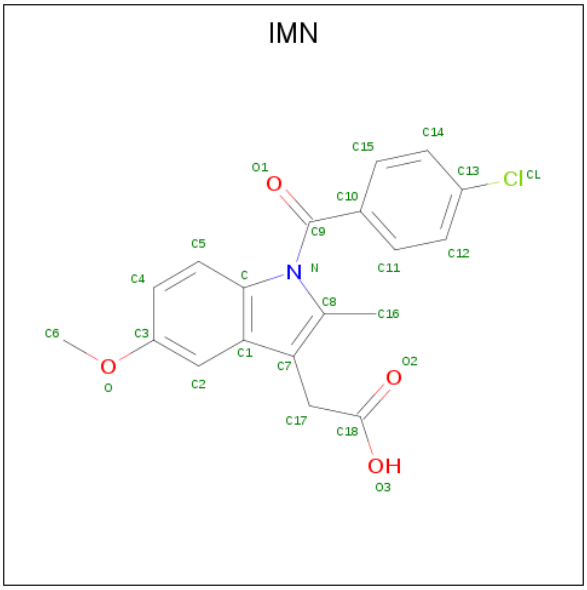
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is INDOMETHACIN (three-letter code: IMN) (formula: $C_{19}H_{16}ClNO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Cl N O 25 19 1 1 4	0	0
3	B	1	Total C Cl N O 25 19 1 1 4	0	0
3	C	1	Total C Cl N O 25 19 1 1 4	0	0
3	D	1	Total C Cl N O 25 19 1 1 4	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Cl 2 2	0	0
4	D	2	Total Cl 2 2	0	0

- Molecule 5 is water.

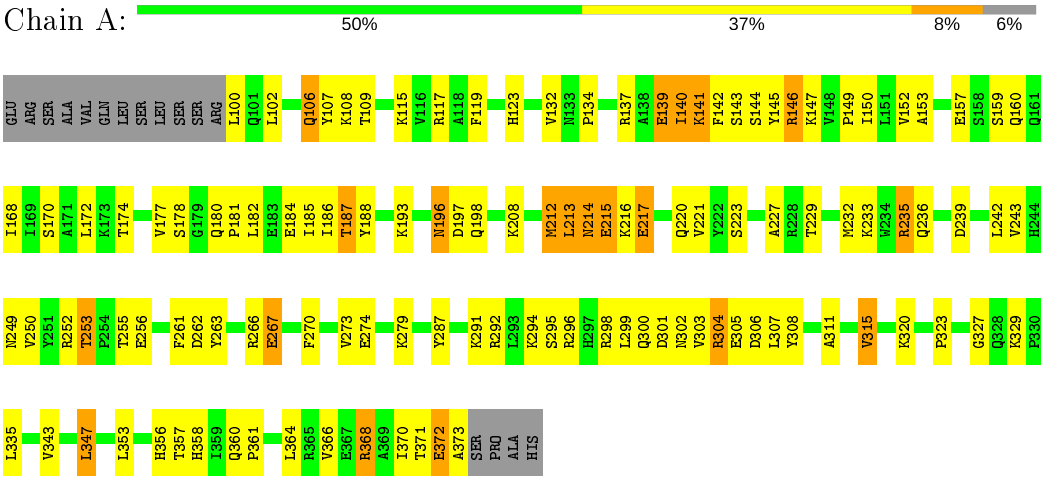
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	23	Total O 23 23	0	0
5	B	26	Total O 26 26	0	0
5	C	21	Total O 21 21	0	0
5	D	18	Total O 18 18	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

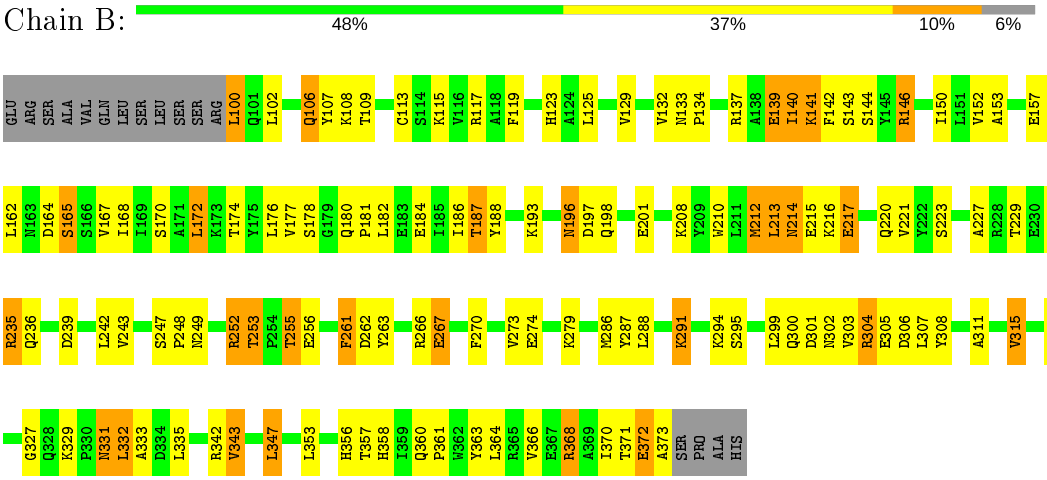
- Molecule 1: membrane-associated prostaglandin E synthase-2

Chain A:



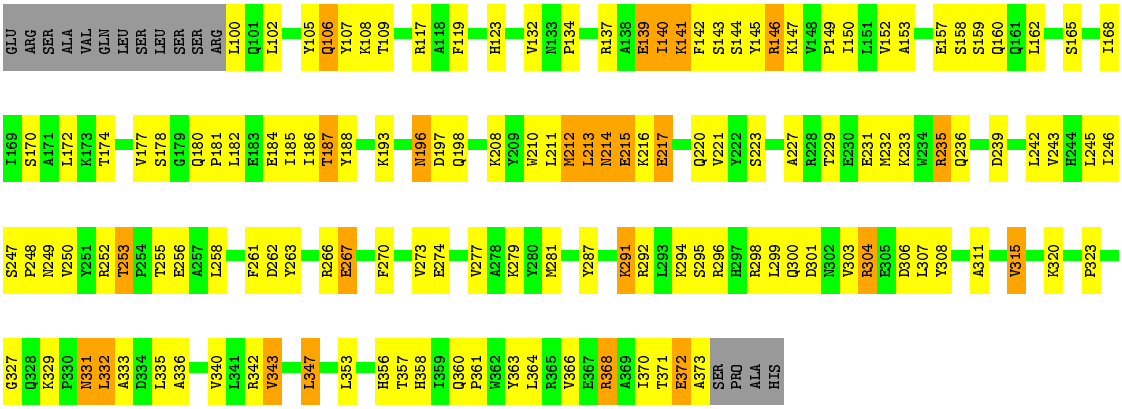
- Molecule 1: membrane-associated prostaglandin E synthase-2

Chain B:



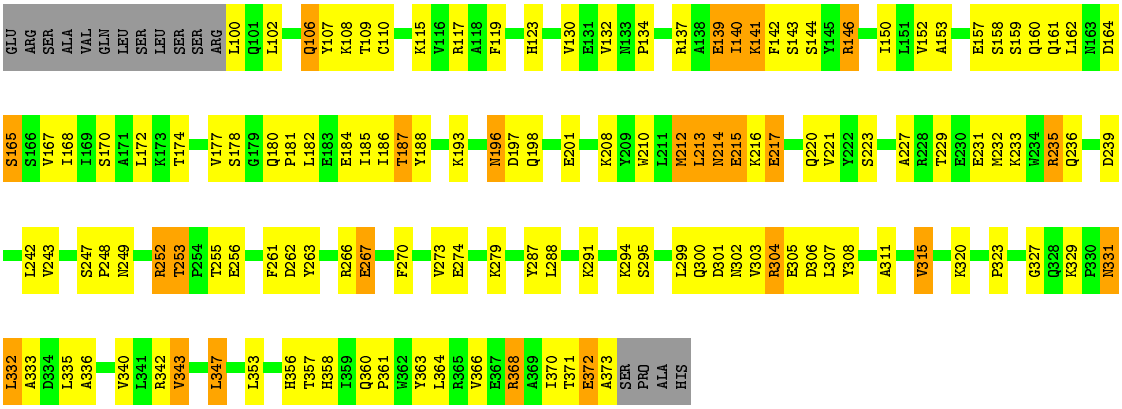
- Molecule 1: membrane-associated prostaglandin E synthase-2

Chain C:



- Molecule 1: membrane-associated prostaglandin E synthase-2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	128.24Å 122.83Å 111.53Å 90.00° 110.60° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.60) 96.6 (20.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.51 (at 2.59Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.251 0.195 , 0.233	Depositor DCC
R_{free} test set	4812 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å^2)	34.3	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.13 , 22.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9064	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, IMN, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.35	0/2266	0.59	1/3070 (0.0%)
1	B	0.36	0/2266	0.60	1/3070 (0.0%)
1	C	0.35	0/2266	0.59	1/3070 (0.0%)
1	D	0.35	0/2266	0.59	1/3070 (0.0%)
All	All	0.35	0/9064	0.59	4/12280 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	107	TYR	N-CA-C	-5.32	96.64	111.00
1	C	107	TYR	N-CA-C	-5.25	96.82	111.00
1	D	107	TYR	N-CA-C	-5.23	96.89	111.00
1	A	107	TYR	N-CA-C	-5.18	97.02	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2214	0	2197	110	0
1	B	2214	0	2197	125	1
1	C	2214	0	2197	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2214	0	2197	119	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
3	A	25	0	15	2	0
3	B	25	0	15	2	0
3	C	25	0	15	2	0
3	D	25	0	15	2	0
4	B	2	0	0	0	0
4	D	2	0	0	0	0
5	A	23	0	0	2	0
5	B	26	0	0	3	0
5	C	21	0	0	6	0
5	D	18	0	0	3	0
All	All	9064	0	8860	462	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (462) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:ARG:HD3	5:B:18:HOH:O	1.58	1.02
1:A:299:LEU:HD23	1:A:303:VAL:HG13	1.50	0.94
1:C:214:ASN:C	1:C:214:ASN:HD22	1.72	0.93
1:D:214:ASN:HD22	1:D:214:ASN:C	1.72	0.92
1:B:299:LEU:HD23	1:B:303:VAL:HG13	1.51	0.92
1:C:299:LEU:HD23	1:C:303:VAL:HG13	1.49	0.92
1:D:299:LEU:HD23	1:D:303:VAL:HG13	1.52	0.90
1:B:214:ASN:HD22	1:B:214:ASN:C	1.73	0.90
1:A:214:ASN:HD22	1:A:214:ASN:C	1.72	0.90
1:A:368:ARG:HD3	5:A:17:HOH:O	1.70	0.90
1:A:170:SER:O	1:A:174:THR:HG23	1.74	0.87
1:C:214:ASN:ND2	1:C:217:GLU:HG2	1.90	0.87
1:B:106:GLN:HE22	1:B:117:ARG:HE	1.23	0.86
1:C:170:SER:O	1:C:174:THR:HG23	1.74	0.86
1:B:214:ASN:ND2	1:B:217:GLU:HG2	1.91	0.84
1:B:170:SER:O	1:B:174:THR:HG23	1.78	0.84
1:D:170:SER:O	1:D:174:THR:HG23	1.78	0.83
1:C:106:GLN:HE22	1:C:117:ARG:HE	1.26	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:ASN:ND2	1:D:217:GLU:HG2	1.94	0.83
1:A:214:ASN:ND2	1:A:217:GLU:HG2	1.93	0.83
1:C:279:LYS:HD3	5:C:82:HOH:O	1.79	0.83
1:D:106:GLN:HE22	1:D:117:ARG:HE	1.26	0.81
1:C:364:LEU:O	1:C:368:ARG:HG2	1.81	0.81
1:A:364:LEU:O	1:A:368:ARG:HG2	1.81	0.81
1:C:140:ILE:HD12	1:C:150:ILE:HD12	1.63	0.80
1:A:106:GLN:HE22	1:A:117:ARG:HE	1.30	0.80
1:A:140:ILE:HD12	1:A:150:ILE:HD12	1.64	0.79
1:B:364:LEU:O	1:B:368:ARG:HG2	1.82	0.79
1:D:364:LEU:O	1:D:368:ARG:HG2	1.82	0.79
1:B:132:VAL:HA	1:B:139:GLU:HG3	1.63	0.78
1:A:239:ASP:HA	1:A:243:VAL:HG13	1.64	0.78
1:D:140:ILE:HD12	1:D:150:ILE:HD12	1.66	0.78
1:D:141:LYS:HD2	1:D:146:ARG:HH12	1.49	0.78
1:C:132:VAL:HA	1:C:139:GLU:HG3	1.65	0.77
1:D:239:ASP:HA	1:D:243:VAL:HG13	1.65	0.77
1:C:239:ASP:HA	1:C:243:VAL:HG13	1.65	0.77
1:C:141:LYS:HD2	1:C:146:ARG:HH12	1.50	0.77
1:A:132:VAL:HA	1:A:139:GLU:HG3	1.66	0.76
1:A:141:LYS:HD2	1:A:146:ARG:HH12	1.50	0.76
1:B:239:ASP:HA	1:B:243:VAL:HG13	1.68	0.76
1:B:140:ILE:HD12	1:B:150:ILE:HD12	1.67	0.76
1:D:132:VAL:HA	1:D:139:GLU:HG3	1.68	0.74
1:C:253:THR:HG22	1:C:256:GLU:HB2	1.69	0.74
1:C:368:ARG:HD3	5:C:19:HOH:O	1.89	0.73
1:D:235:ARG:HH21	1:D:235:ARG:HG2	1.53	0.73
1:B:141:LYS:HD2	1:B:146:ARG:HH12	1.54	0.72
1:D:253:THR:HG22	1:D:256:GLU:HB2	1.70	0.72
1:B:177:VAL:HG21	1:B:213:LEU:HD11	1.71	0.72
1:A:253:THR:HG22	1:A:256:GLU:HB2	1.72	0.72
1:A:214:ASN:HB2	1:B:215:GLU:OE1	1.89	0.71
1:A:253:THR:HG22	1:A:256:GLU:H	1.55	0.71
1:D:235:ARG:HD2	1:D:332:LEU:HB3	1.73	0.71
1:D:235:ARG:NH2	1:D:235:ARG:HG2	2.06	0.71
1:A:235:ARG:HH21	1:A:235:ARG:HG2	1.56	0.70
1:B:253:THR:HG22	1:B:256:GLU:H	1.55	0.70
1:D:368:ARG:HD3	5:D:482:HOH:O	1.89	0.70
1:A:177:VAL:HG21	1:A:213:LEU:HD11	1.74	0.70
1:C:253:THR:HG22	1:C:256:GLU:H	1.56	0.70
1:B:182:LEU:O	1:B:186:ILE:HG23	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:VAL:HG21	1:D:213:LEU:HD11	1.73	0.70
1:D:165:SER:HB3	5:D:480:HOH:O	1.92	0.69
1:D:182:LEU:O	1:D:186:ILE:HG23	1.93	0.69
1:C:214:ASN:C	1:C:214:ASN:ND2	2.46	0.69
1:C:182:LEU:O	1:C:186:ILE:HG23	1.93	0.69
1:B:177:VAL:CG2	1:B:213:LEU:HD11	2.22	0.69
1:C:137:ARG:O	1:C:141:LYS:HD3	1.93	0.68
1:A:235:ARG:HD2	1:A:332:LEU:HB3	1.74	0.68
1:C:263:TYR:O	1:C:267:GLU:HB2	1.94	0.68
1:B:235:ARG:NH2	1:B:235:ARG:HG2	2.08	0.68
1:B:253:THR:HG22	1:B:256:GLU:HB2	1.75	0.68
1:B:249:ASN:ND2	1:B:303:VAL:HG12	2.09	0.68
1:B:235:ARG:HD2	1:B:332:LEU:HB3	1.76	0.68
1:D:249:ASN:ND2	1:D:303:VAL:HG12	2.09	0.68
1:B:235:ARG:HG2	1:B:235:ARG:HH21	1.58	0.68
1:A:177:VAL:CG2	1:A:213:LEU:HD11	2.24	0.68
1:A:182:LEU:O	1:A:186:ILE:HG23	1.93	0.68
1:C:258:LEU:HA	5:C:82:HOH:O	1.94	0.68
1:D:177:VAL:CG2	1:D:213:LEU:HD11	2.25	0.67
1:A:137:ARG:O	1:A:141:LYS:HD3	1.94	0.67
1:A:263:TYR:O	1:A:267:GLU:HB2	1.94	0.67
1:C:140:ILE:CD1	1:C:150:ILE:HD12	2.25	0.67
1:C:235:ARG:HD2	1:C:332:LEU:HB3	1.75	0.67
1:A:140:ILE:CD1	1:A:150:ILE:HD12	2.24	0.67
1:C:214:ASN:HB2	1:D:215:GLU:OE1	1.95	0.66
1:C:174:THR:HG21	1:C:212:MET:H	1.60	0.66
1:D:311:ALA:O	1:D:315:VAL:HG13	1.95	0.66
1:D:253:THR:HG22	1:D:256:GLU:H	1.59	0.66
1:C:177:VAL:HG21	1:C:213:LEU:HD11	1.78	0.66
1:C:235:ARG:HG2	1:C:235:ARG:HH21	1.61	0.65
1:B:263:TYR:O	1:B:267:GLU:HB2	1.96	0.65
1:C:248:PRO:HB2	1:C:303:VAL:HG11	1.77	0.65
1:C:177:VAL:CG2	1:C:213:LEU:HD11	2.26	0.65
1:C:235:ARG:HG2	1:C:235:ARG:NH2	2.11	0.65
1:D:110:CYS:SG	5:D:479:HOH:O	2.54	0.65
1:A:235:ARG:HG2	1:A:235:ARG:NH2	2.09	0.65
1:B:140:ILE:CD1	1:B:150:ILE:HD12	2.27	0.65
1:B:214:ASN:ND2	1:B:214:ASN:C	2.48	0.65
1:A:187:THR:HG23	1:B:229:THR:HG21	1.79	0.64
1:B:311:ALA:O	1:B:315:VAL:HG13	1.98	0.64
1:A:174:THR:HG21	1:A:212:MET:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:ASN:HD21	1:C:217:GLU:H	1.46	0.64
1:D:214:ASN:ND2	1:D:214:ASN:C	2.46	0.64
1:A:366:VAL:O	1:A:370:ILE:HG13	1.99	0.63
1:C:249:ASN:ND2	1:C:303:VAL:HG12	2.14	0.63
1:D:140:ILE:CD1	1:D:150:ILE:HD12	2.28	0.63
1:D:263:TYR:O	1:D:267:GLU:HB2	1.98	0.63
1:C:304:ARG:HG3	1:C:308:TYR:CZ	2.34	0.63
1:C:331:ASN:C	1:C:331:ASN:HD22	2.02	0.62
1:D:331:ASN:C	1:D:331:ASN:HD22	2.02	0.62
1:B:137:ARG:O	1:B:141:LYS:HD3	1.99	0.62
1:B:174:THR:HG21	1:B:212:MET:H	1.64	0.62
1:B:214:ASN:HD21	1:B:217:GLU:H	1.47	0.62
1:C:187:THR:HG23	1:D:229:THR:HG21	1.82	0.62
1:A:331:ASN:HD22	1:A:331:ASN:C	2.02	0.62
1:A:180:GLN:HG3	1:A:181:PRO:HD2	1.82	0.62
1:A:249:ASN:ND2	1:A:303:VAL:HG12	2.15	0.62
1:B:331:ASN:HD22	1:B:331:ASN:C	2.02	0.62
1:A:214:ASN:ND2	1:A:214:ASN:C	2.46	0.61
1:D:174:THR:HG21	1:D:212:MET:H	1.66	0.61
1:A:273:VAL:HG13	1:A:274:GLU:H	1.65	0.61
1:B:214:ASN:ND2	1:B:217:GLU:H	1.99	0.61
1:D:137:ARG:O	1:D:141:LYS:HD3	2.01	0.61
1:D:157:GLU:CD	1:D:157:GLU:H	2.05	0.60
1:C:253:THR:CG2	1:C:256:GLU:H	2.15	0.60
1:C:273:VAL:HG13	1:C:274:GLU:H	1.66	0.60
1:A:304:ARG:HG3	1:A:308:TYR:CZ	2.37	0.60
1:C:217:GLU:O	1:C:221:VAL:HG13	2.01	0.60
1:A:217:GLU:O	1:A:221:VAL:HG13	2.01	0.60
1:D:273:VAL:HG13	1:D:274:GLU:H	1.67	0.60
1:D:214:ASN:HD21	1:D:217:GLU:H	1.49	0.59
1:B:157:GLU:H	1:B:157:GLU:CD	2.05	0.59
1:C:311:ALA:O	1:C:315:VAL:HG13	2.01	0.59
1:B:366:VAL:O	1:B:370:ILE:HG13	2.01	0.59
1:D:214:ASN:ND2	1:D:217:GLU:H	2.00	0.59
1:A:311:ALA:O	1:A:315:VAL:HG13	2.02	0.59
1:C:157:GLU:CD	1:C:157:GLU:H	2.06	0.59
1:B:262:ASP:HB2	1:B:279:LYS:HE2	1.85	0.59
1:B:273:VAL:HG13	1:B:274:GLU:H	1.68	0.59
1:D:304:ARG:HG3	1:D:308:TYR:CZ	2.37	0.59
1:D:357:THR:O	1:D:358:HIS:HB2	2.03	0.59
1:C:180:GLN:HG3	1:C:181:PRO:HD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:GLU:O	1:D:221:VAL:HG13	2.02	0.58
1:A:214:ASN:HD21	1:A:217:GLU:H	1.51	0.58
1:B:217:GLU:O	1:B:221:VAL:HG13	2.03	0.58
1:B:180:GLN:HG3	1:B:181:PRO:HD2	1.85	0.58
1:B:304:ARG:HG3	1:B:308:TYR:CZ	2.38	0.58
1:A:357:THR:O	1:A:358:HIS:HB2	2.04	0.58
1:C:162:LEU:HB2	1:C:168:ILE:HG12	1.85	0.58
1:A:300:GLN:HG3	1:A:306:ASP:OD1	2.04	0.58
1:B:357:THR:O	1:B:358:HIS:HB2	2.04	0.58
1:A:248:PRO:HB2	1:A:303:VAL:HG11	1.84	0.58
1:A:253:THR:CG2	1:A:256:GLU:H	2.17	0.58
1:D:235:ARG:CG	1:D:235:ARG:HH21	2.16	0.58
1:C:366:VAL:O	1:C:370:ILE:HG13	2.04	0.57
1:D:188:TYR:CD1	1:D:212:MET:HG2	2.39	0.57
1:B:235:ARG:HH21	1:B:235:ARG:CG	2.17	0.57
1:B:188:TYR:CD1	1:B:212:MET:HG2	2.40	0.57
1:C:262:ASP:HB2	1:C:279:LYS:HE2	1.85	0.57
1:D:248:PRO:HB2	1:D:303:VAL:HG11	1.85	0.57
1:D:106:GLN:NE2	1:D:117:ARG:HE	1.99	0.57
1:A:214:ASN:ND2	1:A:217:GLU:H	2.03	0.57
1:B:106:GLN:NE2	1:B:117:ARG:HE	1.98	0.57
1:C:214:ASN:ND2	1:C:217:GLU:H	2.01	0.57
1:A:235:ARG:HH21	1:A:235:ARG:CG	2.18	0.56
1:D:180:GLN:HG3	1:D:181:PRO:HD2	1.87	0.56
1:B:170:SER:OG	1:B:235:ARG:NH1	2.39	0.56
1:D:253:THR:CG2	1:D:256:GLU:H	2.19	0.56
1:A:323:PRO:HG2	1:A:327:GLY:O	2.06	0.56
1:D:141:LYS:HD2	1:D:146:ARG:NH1	2.20	0.56
1:A:157:GLU:H	1:A:157:GLU:CD	2.09	0.56
1:B:248:PRO:HB2	1:B:303:VAL:HG11	1.86	0.55
1:D:262:ASP:HB2	1:D:279:LYS:HE2	1.87	0.55
1:A:170:SER:OG	1:A:235:ARG:NH1	2.40	0.55
1:C:357:THR:O	1:C:358:HIS:HB2	2.07	0.55
1:D:366:VAL:O	1:D:370:ILE:HG13	2.06	0.55
1:A:298:ARG:NH1	1:B:201:GLU:HG3	2.21	0.55
1:B:300:GLN:HG3	1:B:306:ASP:OD1	2.07	0.55
1:D:184:GLU:O	1:D:187:THR:HB	2.06	0.55
1:A:106:GLN:NE2	1:A:117:ARG:HE	2.03	0.55
1:B:184:GLU:O	1:B:187:THR:HB	2.06	0.55
1:C:235:ARG:CG	1:C:235:ARG:HH21	2.19	0.55
1:A:162:LEU:HB2	1:A:168:ILE:HG12	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:TYR:CD1	1:A:212:MET:HG2	2.42	0.54
1:A:262:ASP:HB2	1:A:279:LYS:HE2	1.88	0.54
1:C:188:TYR:CD1	1:C:212:MET:HG2	2.42	0.54
1:D:300:GLN:HG3	1:D:306:ASP:OD1	2.08	0.54
1:A:360:GLN:HB3	1:A:361:PRO:HD3	1.90	0.54
1:D:331:ASN:HD21	1:D:333:ALA:HB3	1.72	0.54
1:B:253:THR:CG2	1:B:256:GLU:H	2.19	0.54
1:B:162:LEU:HB2	1:B:168:ILE:HG12	1.89	0.54
1:C:360:GLN:HB3	1:C:361:PRO:HD3	1.89	0.54
1:C:106:GLN:NE2	1:C:117:ARG:HE	2.01	0.53
1:C:170:SER:OG	1:C:235:ARG:NH1	2.40	0.53
1:C:177:VAL:HG23	1:C:178:SER:N	2.23	0.53
1:C:181:PRO:HG2	1:C:184:GLU:CD	2.28	0.53
1:A:119:PHE:O	1:A:123:HIS:HD2	1.92	0.53
1:A:177:VAL:HG23	1:A:178:SER:N	2.24	0.53
1:C:239:ASP:HA	1:C:243:VAL:CG1	2.35	0.53
1:B:132:VAL:HA	1:B:139:GLU:CG	2.34	0.53
1:A:132:VAL:HA	1:A:139:GLU:CG	2.38	0.52
1:C:300:GLN:HG3	1:C:306:ASP:OD1	2.09	0.52
1:B:119:PHE:O	1:B:123:HIS:HD2	1.91	0.52
1:D:239:ASP:HA	1:D:243:VAL:CG1	2.38	0.52
1:C:132:VAL:HA	1:C:139:GLU:CG	2.38	0.52
1:C:323:PRO:HG2	1:C:327:GLY:O	2.09	0.52
1:D:170:SER:OG	1:D:235:ARG:NH1	2.43	0.52
1:D:177:VAL:HG23	1:D:178:SER:N	2.23	0.52
1:D:294:LYS:HD2	1:D:303:VAL:HG22	1.91	0.52
1:C:134:PRO:HG3	3:C:379:IMN:H61	1.91	0.52
1:C:153:ALA:O	1:C:159:SER:HA	2.09	0.51
1:D:162:LEU:N	1:D:162:LEU:HD23	2.25	0.51
1:C:347:LEU:HD21	3:C:379:IMN:CL	2.48	0.51
1:D:162:LEU:HB2	1:D:168:ILE:HG12	1.92	0.51
1:C:298:ARG:NH1	1:D:201:GLU:HG3	2.26	0.51
1:B:162:LEU:N	1:B:162:LEU:HD23	2.25	0.51
1:B:177:VAL:HG23	1:B:178:SER:N	2.25	0.51
1:B:233:LYS:HB2	5:B:51:HOH:O	2.10	0.51
1:C:141:LYS:HD2	1:C:146:ARG:NH1	2.22	0.51
1:C:162:LEU:N	1:C:162:LEU:HD23	2.25	0.51
1:B:141:LYS:HD2	1:B:146:ARG:NH1	2.22	0.51
1:C:196:ASN:ND2	1:C:197:ASP:H	2.08	0.51
1:A:184:GLU:O	1:A:187:THR:HB	2.11	0.51
1:B:165:SER:HB3	5:B:10:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:LYS:HD2	1:B:303:VAL:HG22	1.91	0.51
1:D:132:VAL:HA	1:D:139:GLU:CG	2.38	0.51
1:A:141:LYS:HD2	1:A:146:ARG:NH1	2.22	0.50
1:A:347:LEU:HD21	3:A:379:IMN:CL	2.48	0.50
1:D:371:THR:C	1:D:373:ALA:H	2.13	0.50
1:A:153:ALA:O	1:A:159:SER:HA	2.11	0.50
1:C:258:LEU:CA	5:C:82:HOH:O	2.57	0.50
1:D:347:LEU:HD21	3:D:476:IMN:CL	2.48	0.50
1:B:371:THR:C	1:B:373:ALA:H	2.14	0.50
1:D:134:PRO:HG2	1:D:270:PHE:CZ	2.47	0.50
1:A:162:LEU:HD23	1:A:162:LEU:N	2.26	0.50
1:C:368:ARG:O	1:C:372:GLU:HB2	2.11	0.50
1:D:140:ILE:O	1:D:140:ILE:HG23	2.11	0.50
1:C:196:ASN:HD22	1:C:197:ASP:H	1.59	0.50
1:B:132:VAL:HG13	1:B:139:GLU:HG2	1.93	0.50
1:B:140:ILE:CG2	1:B:140:ILE:O	2.60	0.50
1:B:140:ILE:HG23	1:B:140:ILE:O	2.10	0.50
1:A:214:ASN:HD21	1:A:216:LYS:HB2	1.77	0.49
1:A:239:ASP:HA	1:A:243:VAL:CG1	2.36	0.49
1:D:214:ASN:HD21	1:D:216:LYS:HB2	1.77	0.49
1:D:262:ASP:O	1:D:266:ARG:HD3	2.11	0.49
1:B:153:ALA:O	1:B:159:SER:HA	2.12	0.49
1:B:331:ASN:HD21	1:B:333:ALA:HB3	1.77	0.49
1:D:153:ALA:O	1:D:159:SER:HA	2.12	0.49
1:A:196:ASN:ND2	1:A:197:ASP:H	2.09	0.49
1:B:142:PHE:CD2	1:B:142:PHE:C	2.86	0.49
1:B:196:ASN:ND2	1:B:197:ASP:H	2.10	0.49
1:B:210:TRP:HD1	1:B:212:MET:HE3	1.78	0.49
1:D:187:THR:HG22	1:D:188:TYR:CD2	2.48	0.49
1:B:214:ASN:HD21	1:B:216:LYS:HB2	1.77	0.49
1:A:187:THR:CG2	1:B:229:THR:HG21	2.42	0.49
1:B:347:LEU:HD21	3:B:381:IMN:CL	2.48	0.49
1:D:140:ILE:O	1:D:140:ILE:CG2	2.60	0.49
1:D:323:PRO:HG2	1:D:327:GLY:O	2.12	0.49
1:B:229:THR:HA	1:B:232:MET:HE2	1.94	0.49
1:D:368:ARG:O	1:D:372:GLU:HB2	2.12	0.49
1:B:239:ASP:HA	1:B:243:VAL:CG1	2.41	0.49
1:C:140:ILE:HD13	1:C:140:ILE:HA	1.69	0.49
1:B:262:ASP:O	1:B:266:ARG:HD3	2.13	0.48
1:C:184:GLU:O	1:C:187:THR:HB	2.13	0.48
1:D:132:VAL:HG13	1:D:139:GLU:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:THR:HG22	1:B:188:TYR:CD2	2.48	0.48
1:D:108:LYS:HG2	1:D:267:GLU:HG3	1.96	0.48
1:D:119:PHE:O	1:D:123:HIS:HD2	1.96	0.48
1:A:134:PRO:HG3	3:A:379:IMN:H61	1.96	0.48
1:A:187:THR:HG22	1:A:188:TYR:CD2	2.49	0.48
1:A:273:VAL:HG13	1:A:274:GLU:N	2.28	0.48
1:A:294:LYS:HD2	1:A:303:VAL:HG22	1.95	0.48
1:B:302:ASN:ND2	1:B:305:GLU:HG2	2.29	0.48
1:A:181:PRO:HG2	1:A:184:GLU:CD	2.33	0.48
1:B:140:ILE:HA	1:B:140:ILE:HD13	1.64	0.48
1:C:273:VAL:HG13	1:C:274:GLU:N	2.29	0.48
1:B:247:SER:HB2	1:B:248:PRO:CD	2.43	0.48
1:D:287:TYR:O	1:D:291:LYS:HG2	2.14	0.48
1:C:371:THR:C	1:C:373:ALA:H	2.17	0.47
1:D:196:ASN:ND2	1:D:197:ASP:H	2.12	0.47
1:C:132:VAL:HG13	1:C:139:GLU:HG2	1.94	0.47
1:A:296:ARG:NH2	1:B:197:ASP:HA	2.29	0.47
1:C:262:ASP:O	1:C:266:ARG:HD3	2.15	0.47
1:C:331:ASN:HD21	1:C:333:ALA:HB3	1.79	0.47
1:D:142:PHE:C	1:D:142:PHE:CD2	2.87	0.47
1:B:125:LEU:HD11	1:B:176:LEU:HD11	1.96	0.47
1:B:181:PRO:HG2	1:B:184:GLU:CD	2.35	0.47
1:B:287:TYR:O	1:B:291:LYS:HG2	2.14	0.47
1:C:294:LYS:HD2	1:C:303:VAL:HG22	1.95	0.47
1:C:304:ARG:HG3	1:C:308:TYR:OH	2.14	0.47
1:D:360:GLN:HB3	1:D:361:PRO:HD3	1.96	0.47
1:A:287:TYR:O	1:A:291:LYS:HG2	2.14	0.47
1:A:140:ILE:HD13	1:A:140:ILE:HA	1.67	0.47
1:A:253:THR:HG22	1:A:256:GLU:CB	2.43	0.47
1:A:108:LYS:HG2	1:A:267:GLU:HG3	1.97	0.47
1:A:371:THR:C	1:A:373:ALA:H	2.17	0.47
1:B:196:ASN:HD22	1:B:197:ASP:H	1.63	0.47
1:C:149:PRO:HD3	5:C:7:HOH:O	2.15	0.47
1:A:140:ILE:O	1:A:140:ILE:HG23	2.14	0.47
1:C:108:LYS:HG2	1:C:267:GLU:HG3	1.97	0.47
1:D:273:VAL:HG13	1:D:274:GLU:N	2.30	0.47
1:A:368:ARG:O	1:A:372:GLU:HB2	2.14	0.47
1:B:273:VAL:HG13	1:B:274:GLU:N	2.29	0.47
1:D:181:PRO:HG2	1:D:184:GLU:CD	2.35	0.47
1:A:141:LYS:HA	1:A:146:ARG:HH22	1.81	0.46
1:C:253:THR:HG22	1:C:256:GLU:CB	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:THR:O	1:D:343:VAL:HG22	2.14	0.46
1:D:302:ASN:ND2	1:D:305:GLU:HG2	2.30	0.46
1:B:249:ASN:HD21	1:B:303:VAL:HG12	1.78	0.46
1:A:196:ASN:HD22	1:A:197:ASP:H	1.62	0.46
1:B:323:PRO:HG2	1:B:327:GLY:O	2.15	0.46
1:B:368:ARG:O	1:B:372:GLU:HB2	2.15	0.46
1:A:262:ASP:O	1:A:266:ARG:HD3	2.15	0.46
1:C:246:ILE:O	1:C:250:VAL:HG22	2.15	0.46
1:A:149:PRO:HD3	5:A:5:HOH:O	2.15	0.46
1:A:140:ILE:CG2	1:A:140:ILE:O	2.64	0.46
1:A:246:ILE:O	1:A:250:VAL:HG22	2.15	0.46
1:B:134:PRO:HG2	1:B:270:PHE:CZ	2.51	0.46
1:A:331:ASN:HD21	1:A:333:ALA:HB3	1.81	0.46
1:B:187:THR:HG22	1:B:188:TYR:CE2	2.51	0.46
1:B:360:GLN:HB3	1:B:361:PRO:HD3	1.98	0.46
1:D:115:LYS:HB3	1:D:115:LYS:HE2	1.70	0.46
1:D:210:TRP:HD1	1:D:212:MET:HE3	1.81	0.45
1:A:247:SER:HB2	1:A:248:PRO:CD	2.46	0.45
1:C:134:PRO:HG2	1:C:270:PHE:CZ	2.52	0.45
1:C:141:LYS:HA	1:C:146:ARG:HH22	1.81	0.45
1:C:247:SER:HB2	1:C:248:PRO:CD	2.46	0.45
1:D:134:PRO:HG3	3:D:476:IMN:H61	1.98	0.45
1:D:174:THR:OG1	1:D:185:ILE:HD13	2.17	0.45
1:D:187:THR:HG22	1:D:188:TYR:CE2	2.52	0.45
1:D:294:LYS:O	1:D:299:LEU:HB2	2.16	0.45
1:C:109:THR:HG22	1:C:263:TYR:CZ	2.52	0.45
1:D:294:LYS:HD2	1:D:303:VAL:CG2	2.46	0.45
1:B:108:LYS:O	1:B:117:ARG:NH2	2.50	0.45
1:C:287:TYR:O	1:C:291:LYS:HG2	2.17	0.45
1:D:152:VAL:HA	1:D:160:GLN:O	2.16	0.45
1:D:331:ASN:C	1:D:331:ASN:ND2	2.69	0.45
1:B:152:VAL:HA	1:B:160:GLN:O	2.16	0.45
1:C:229:THR:HA	1:C:232:MET:HE2	1.98	0.45
1:B:223:SER:HB2	1:B:227:ALA:CB	2.46	0.45
1:C:142:PHE:CD2	1:C:142:PHE:C	2.90	0.45
1:B:342:ARG:HA	1:B:363:TYR:OH	2.17	0.45
1:C:331:ASN:ND2	1:C:331:ASN:C	2.69	0.45
1:C:187:THR:HG22	1:C:188:TYR:CD2	2.52	0.44
1:C:108:LYS:O	1:C:117:ARG:NH2	2.51	0.44
1:D:342:ARG:HA	1:D:363:TYR:OH	2.18	0.44
1:A:109:THR:HG22	1:A:263:TYR:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:LYS:O	1:C:299:LEU:HB2	2.17	0.44
1:D:130:VAL:HG22	1:D:130:VAL:O	2.17	0.44
1:B:108:LYS:HG2	1:B:267:GLU:HG3	1.99	0.44
1:B:368:ARG:HG3	1:B:368:ARG:HH21	1.83	0.44
1:C:181:PRO:O	1:C:185:ILE:HG13	2.17	0.44
1:C:217:GLU:O	1:C:220:GLN:HB3	2.18	0.44
1:B:141:LYS:HA	1:B:146:ARG:HH22	1.83	0.44
1:B:223:SER:HB2	1:B:227:ALA:HB2	2.00	0.44
1:D:196:ASN:HD22	1:D:197:ASP:H	1.65	0.44
1:D:252:ARG:HH11	1:D:252:ARG:CG	2.31	0.44
1:A:294:LYS:O	1:A:299:LEU:HB2	2.17	0.43
1:B:210:TRP:CD1	1:B:212:MET:HE3	2.53	0.43
1:C:119:PHE:O	1:C:123:HIS:HD2	2.00	0.43
1:D:331:ASN:ND2	1:D:333:ALA:H	2.16	0.43
1:C:140:ILE:O	1:C:140:ILE:CG2	2.66	0.43
1:C:187:THR:CG2	1:D:229:THR:HG21	2.48	0.43
1:D:253:THR:HG22	1:D:256:GLU:CB	2.45	0.43
1:A:181:PRO:O	1:A:185:ILE:HG13	2.19	0.43
1:A:253:THR:HB	1:A:256:GLU:OE2	2.18	0.43
1:C:140:ILE:O	1:C:140:ILE:HG23	2.18	0.43
1:C:217:GLU:H	1:C:217:GLU:HG2	1.59	0.43
1:C:253:THR:HB	1:C:256:GLU:OE2	2.19	0.43
1:D:137:ARG:HB2	1:D:141:LYS:HE3	2.01	0.43
1:D:164:ASP:HB3	1:D:167:VAL:HG23	2.00	0.43
1:D:217:GLU:O	1:D:220:GLN:HB3	2.18	0.43
1:D:247:SER:HB2	1:D:248:PRO:CD	2.48	0.43
1:A:152:VAL:HA	1:A:160:GLN:O	2.19	0.43
1:A:187:THR:HG22	1:A:188:TYR:CE2	2.53	0.43
1:B:331:ASN:ND2	1:B:331:ASN:C	2.70	0.43
1:D:108:LYS:O	1:D:117:ARG:NH2	2.52	0.43
1:A:323:PRO:HD2	1:A:327:GLY:O	2.18	0.43
1:B:134:PRO:HG3	3:B:381:IMN:H61	2.01	0.43
1:B:304:ARG:HG3	1:B:308:TYR:OH	2.19	0.43
1:A:139:GLU:H	1:A:139:GLU:CD	2.22	0.43
1:A:331:ASN:C	1:A:331:ASN:ND2	2.69	0.43
1:C:258:LEU:HD23	5:C:82:HOH:O	2.18	0.43
1:D:141:LYS:HA	1:D:146:ARG:HH22	1.83	0.43
1:A:132:VAL:HG13	1:A:139:GLU:HG2	2.01	0.43
1:A:223:SER:HB2	1:A:227:ALA:HB2	2.00	0.43
1:B:115:LYS:HB3	1:B:115:LYS:HE2	1.71	0.43
1:D:141:LYS:HA	1:D:146:ARG:NH2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:HIS:N	1:B:356:HIS:CD2	2.87	0.42
1:A:217:GLU:O	1:A:220:GLN:HB3	2.20	0.42
1:D:249:ASN:HD21	1:D:303:VAL:HG12	1.82	0.42
1:B:137:ARG:HB2	1:B:141:LYS:HE3	2.02	0.42
1:B:252:ARG:HH11	1:B:252:ARG:CG	2.31	0.42
1:B:294:LYS:O	1:B:299:LEU:HB2	2.18	0.42
1:C:296:ARG:NH2	1:D:197:ASP:HA	2.34	0.42
1:D:164:ASP:HB3	1:D:167:VAL:CG2	2.49	0.42
1:D:336:ALA:O	1:D:340:VAL:HG23	2.20	0.42
1:B:294:LYS:HD2	1:B:303:VAL:CG2	2.49	0.42
1:C:132:VAL:O	1:C:134:PRO:HD3	2.20	0.42
1:C:152:VAL:HA	1:C:160:GLN:O	2.20	0.42
1:D:229:THR:HA	1:D:232:MET:HE2	2.00	0.42
1:B:261:PHE:HE2	1:B:286:MET:HG3	1.84	0.42
1:C:141:LYS:HA	1:C:146:ARG:NH2	2.35	0.42
1:C:223:SER:HB2	1:C:227:ALA:HB2	1.99	0.42
1:A:145:TYR:CZ	1:A:147:LYS:HB2	2.54	0.42
1:A:134:PRO:HG2	1:A:270:PHE:CZ	2.54	0.42
1:A:302:ASN:ND2	1:A:305:GLU:HG2	2.34	0.42
1:B:141:LYS:HA	1:B:146:ARG:NH2	2.34	0.42
1:C:187:THR:HG22	1:C:188:TYR:CE2	2.55	0.42
1:C:214:ASN:HD21	1:C:216:LYS:HB2	1.85	0.42
1:C:336:ALA:O	1:C:340:VAL:HG23	2.20	0.42
1:B:231:GLU:HG3	1:B:232:MET:N	2.35	0.42
1:C:210:TRP:HD1	1:C:212:MET:HE3	1.85	0.41
1:D:161:GLN:C	1:D:162:LEU:HD23	2.40	0.41
1:C:215:GLU:OE1	1:D:214:ASN:HB2	2.20	0.41
1:D:356:HIS:N	1:D:356:HIS:CD2	2.88	0.41
1:A:115:LYS:HB3	1:A:115:LYS:HE2	1.71	0.41
1:A:108:LYS:O	1:A:117:ARG:NH2	2.53	0.41
1:A:142:PHE:CD2	1:A:142:PHE:C	2.93	0.41
1:B:177:VAL:HG21	1:B:213:LEU:CD1	2.47	0.41
1:C:174:THR:HG22	1:C:211:LEU:HB3	2.02	0.41
1:D:223:SER:HB2	1:D:227:ALA:HB2	2.02	0.41
1:C:109:THR:O	1:C:343:VAL:HG22	2.20	0.41
1:A:331:ASN:ND2	1:A:333:ALA:H	2.18	0.41
1:A:368:ARG:HH21	1:A:368:ARG:HG3	1.85	0.41
1:A:141:LYS:HA	1:A:146:ARG:NH2	2.35	0.41
1:D:231:GLU:HG3	1:D:232:MET:N	2.35	0.41
1:A:245:LEU:O	1:A:249:ASN:HB2	2.20	0.41
1:B:161:GLN:C	1:B:162:LEU:HD23	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:ARG:HA	1:C:363:TYR:OH	2.20	0.41
1:A:215:GLU:OE1	1:B:214:ASN:HB2	2.20	0.41
1:C:294:LYS:HD2	1:C:303:VAL:CG2	2.50	0.41
1:B:129:VAL:O	1:B:129:VAL:CG2	2.69	0.41
1:B:217:GLU:O	1:B:220:GLN:HB3	2.21	0.41
1:B:368:ARG:H	1:B:368:ARG:HG2	1.55	0.41
1:B:100:LEU:HD21	1:B:153:ALA:HB1	2.03	0.41
1:C:231:GLU:HG3	1:C:232:MET:N	2.36	0.41
1:C:331:ASN:ND2	1:C:333:ALA:H	2.18	0.41
1:A:137:ARG:HB2	1:A:141:LYS:HE3	2.03	0.41
1:B:109:THR:O	1:B:343:VAL:HG22	2.21	0.41
1:C:356:HIS:N	1:C:356:HIS:CD2	2.89	0.41
1:A:229:THR:HA	1:A:232:MET:HE2	2.03	0.40
1:A:356:HIS:N	1:A:356:HIS:CD2	2.88	0.40
1:C:145:TYR:CE1	1:C:147:LYS:HB2	2.57	0.40
1:D:139:GLU:H	1:D:139:GLU:CD	2.24	0.40
1:B:288:LEU:O	1:B:291:LYS:HB2	2.21	0.40
1:B:331:ASN:ND2	1:B:333:ALA:H	2.19	0.40
1:C:139:GLU:H	1:C:139:GLU:CD	2.23	0.40
1:C:245:LEU:O	1:C:249:ASN:HB2	2.21	0.40
1:C:277:VAL:HG13	1:C:281:MET:HG3	2.02	0.40
1:D:210:TRP:CD1	1:D:212:MET:HE3	2.56	0.40
1:B:133:ASN:HA	1:B:134:PRO:HD2	1.96	0.40
1:C:210:TRP:CD1	1:C:212:MET:HE3	2.57	0.40
1:D:109:THR:HG22	1:D:263:TYR:CZ	2.56	0.40
1:B:164:ASP:HB3	1:B:167:VAL:CG2	2.51	0.40
1:B:255:THR:HB	1:C:141:LYS:NZ	2.37	0.40
1:D:288:LEU:O	1:D:291:LYS:HB2	2.21	0.40
1:D:368:ARG:HG2	1:D:368:ARG:H	1.57	0.40
1:A:296:ARG:HD2	1:B:197:ASP:C	2.42	0.40
1:B:106:GLN:HB2	1:B:113:CYS:SG	2.61	0.40
1:B:168:ILE:O	1:B:172:LEU:HB2	2.22	0.40
1:C:105:TYR:HE1	1:C:152:VAL:HG13	1.86	0.40
1:D:368:ARG:HG3	1:D:368:ARG:HH21	1.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:SER:OG	1:B:321:ASP:OD2[2_556]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	272/290 (94%)	262 (96%)	10 (4%)	0	100	100
1	B	272/290 (94%)	264 (97%)	8 (3%)	0	100	100
1	C	272/290 (94%)	263 (97%)	9 (3%)	0	100	100
1	D	272/290 (94%)	263 (97%)	9 (3%)	0	100	100
All	All	1088/1160 (94%)	1052 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	233/247 (94%)	187 (80%)	46 (20%)	1	2
1	B	233/247 (94%)	187 (80%)	46 (20%)	1	2
1	C	233/247 (94%)	185 (79%)	48 (21%)	1	2
1	D	233/247 (94%)	187 (80%)	46 (20%)	1	2
All	All	932/988 (94%)	746 (80%)	186 (20%)	1	2

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	LEU
1	A	102	LEU

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Mol	Chain	Res	Type
1	A	106	GLN
1	A	139	GLU
1	A	140	ILE
1	A	141	LYS
1	A	143	SER
1	A	144	SER
1	A	146	ARG
1	A	165	SER
1	A	172	LEU
1	A	187	THR
1	A	193	LYS
1	A	196	ASN
1	A	198	GLN
1	A	208	LYS
1	A	212	MET
1	A	213	LEU
1	A	214	ASN
1	A	215	GLU
1	A	217	GLU
1	A	233	LYS
1	A	235	ARG
1	A	236	GLN
1	A	242	LEU
1	A	252	ARG
1	A	253	THR
1	A	255	THR
1	A	261	PHE
1	A	267	GLU
1	A	292	ARG
1	A	295	SER
1	A	301	ASP
1	A	304	ARG
1	A	307	LEU
1	A	315	VAL
1	A	320	LYS
1	A	329	LYS
1	A	331	ASN
1	A	332	LEU
1	A	335	LEU
1	A	343	VAL
1	A	347	LEU
1	A	353	LEU

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Mol	Chain	Res	Type
1	A	368	ARG
1	A	372	GLU
1	B	100	LEU
1	B	102	LEU
1	B	106	GLN
1	B	139	GLU
1	B	140	ILE
1	B	141	LYS
1	B	143	SER
1	B	144	SER
1	B	146	ARG
1	B	158	SER
1	B	165	SER
1	B	172	LEU
1	B	187	THR
1	B	193	LYS
1	B	196	ASN
1	B	198	GLN
1	B	208	LYS
1	B	212	MET
1	B	213	LEU
1	B	214	ASN
1	B	217	GLU
1	B	233	LYS
1	B	235	ARG
1	B	236	GLN
1	B	242	LEU
1	B	252	ARG
1	B	253	THR
1	B	255	THR
1	B	261	PHE
1	B	267	GLU
1	B	291	LYS
1	B	295	SER
1	B	301	ASP
1	B	304	ARG
1	B	307	LEU
1	B	315	VAL
1	B	320	LYS
1	B	329	LYS
1	B	331	ASN
1	B	332	LEU

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Mol	Chain	Res	Type
1	B	335	LEU
1	B	343	VAL
1	B	347	LEU
1	B	353	LEU
1	B	368	ARG
1	B	372	GLU
1	C	100	LEU
1	C	102	LEU
1	C	106	GLN
1	C	139	GLU
1	C	140	ILE
1	C	141	LYS
1	C	143	SER
1	C	144	SER
1	C	146	ARG
1	C	158	SER
1	C	165	SER
1	C	172	LEU
1	C	187	THR
1	C	193	LYS
1	C	196	ASN
1	C	198	GLN
1	C	208	LYS
1	C	212	MET
1	C	213	LEU
1	C	214	ASN
1	C	215	GLU
1	C	217	GLU
1	C	233	LYS
1	C	235	ARG
1	C	236	GLN
1	C	242	LEU
1	C	252	ARG
1	C	253	THR
1	C	255	THR
1	C	261	PHE
1	C	267	GLU
1	C	291	LYS
1	C	292	ARG
1	C	295	SER
1	C	301	ASP
1	C	304	ARG

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Mol	Chain	Res	Type
1	C	307	LEU
1	C	315	VAL
1	C	320	LYS
1	C	329	LYS
1	C	331	ASN
1	C	332	LEU
1	C	335	LEU
1	C	343	VAL
1	C	347	LEU
1	C	353	LEU
1	C	368	ARG
1	C	372	GLU
1	D	100	LEU
1	D	102	LEU
1	D	106	GLN
1	D	139	GLU
1	D	140	ILE
1	D	141	LYS
1	D	143	SER
1	D	144	SER
1	D	146	ARG
1	D	158	SER
1	D	165	SER
1	D	172	LEU
1	D	187	THR
1	D	193	LYS
1	D	196	ASN
1	D	198	GLN
1	D	208	LYS
1	D	212	MET
1	D	213	LEU
1	D	214	ASN
1	D	215	GLU
1	D	217	GLU
1	D	233	LYS
1	D	235	ARG
1	D	236	GLN
1	D	242	LEU
1	D	252	ARG
1	D	253	THR
1	D	255	THR
1	D	261	PHE

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Mol	Chain	Res	Type
1	D	267	GLU
1	D	295	SER
1	D	301	ASP
1	D	304	ARG
1	D	307	LEU
1	D	315	VAL
1	D	320	LYS
1	D	329	LYS
1	D	331	ASN
1	D	332	LEU
1	D	335	LEU
1	D	343	VAL
1	D	347	LEU
1	D	353	LEU
1	D	368	ARG
1	D	372	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	123	HIS
1	A	161	GLN
1	A	196	ASN
1	A	214	ASN
1	A	219	GLN
1	A	236	GLN
1	A	244	HIS
1	A	297	HIS
1	A	331	ASN
1	A	356	HIS
1	B	106	GLN
1	B	123	HIS
1	B	154	GLN
1	B	196	ASN
1	B	214	ASN
1	B	219	GLN
1	B	236	GLN
1	B	244	HIS
1	B	297	HIS
1	B	331	ASN
1	B	356	HIS

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Mol	Chain	Res	Type
1	C	106	GLN
1	C	123	HIS
1	C	196	ASN
1	C	214	ASN
1	C	219	GLN
1	C	236	GLN
1	C	244	HIS
1	C	297	HIS
1	C	331	ASN
1	C	356	HIS
1	D	106	GLN
1	D	123	HIS
1	D	154	GLN
1	D	196	ASN
1	D	214	ASN
1	D	219	GLN
1	D	236	GLN
1	D	244	HIS
1	D	297	HIS
1	D	331	ASN
1	D	356	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ACT	A	378	-	1,3,3	1.67	0	0,3,3	0.00	-
2	ACT	C	378	-	1,3,3	1.79	0	0,3,3	0.00	-
3	IMN	B	381	-	21,27,27	2.97	12 (57%)	26,39,39	3.52	12 (46%)
2	ACT	B	379	-	1,3,3	1.51	0	0,3,3	0.00	-
2	ACT	D	477	-	1,3,3	1.91	0	0,3,3	0.00	-
3	IMN	A	379	-	21,27,27	2.96	15 (71%)	26,39,39	3.53	12 (46%)
3	IMN	C	379	-	21,27,27	2.92	13 (61%)	26,39,39	3.56	12 (46%)
3	IMN	D	476	-	21,27,27	2.89	12 (57%)	26,39,39	3.52	12 (46%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IMN	A	379	-	-	0/8/14/14	0/3/3/3
3	IMN	D	476	-	-	0/8/14/14	0/3/3/3
3	IMN	B	381	-	-	0/8/14/14	0/3/3/3
3	IMN	C	379	-	-	0/8/14/14	0/3/3/3

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	379	IMN	C8-C7	5.93	1.51	1.39
3	B	381	IMN	C8-C7	5.84	1.51	1.39
3	B	381	IMN	C10-C9	5.65	1.59	1.50
3	A	379	IMN	C8-C7	5.60	1.50	1.39
3	D	476	IMN	C8-C7	5.59	1.50	1.39
3	C	379	IMN	C10-C9	5.17	1.58	1.50
3	D	476	IMN	C10-C9	5.13	1.58	1.50
3	A	379	IMN	C10-C9	4.87	1.58	1.50
3	A	379	IMN	C11-C10	3.88	1.45	1.39
3	D	476	IMN	C15-C14	3.86	1.45	1.38
3	B	381	IMN	C15-C10	3.79	1.45	1.39
3	B	381	IMN	C11-C10	3.76	1.45	1.39
3	A	379	IMN	C12-C11	3.74	1.45	1.38
3	A	379	IMN	C15-C14	3.74	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	379	IMN	C11-C10	3.71	1.45	1.39
3	C	379	IMN	C12-C11	3.69	1.45	1.38
3	D	476	IMN	C15-C10	3.65	1.45	1.39
3	B	381	IMN	C15-C14	3.61	1.45	1.38
3	B	381	IMN	C12-C11	3.58	1.45	1.38
3	D	476	IMN	C11-C10	3.57	1.45	1.39
3	D	476	IMN	C2-C3	3.57	1.43	1.37
3	A	379	IMN	C15-C10	3.54	1.45	1.39
3	B	381	IMN	C8-N	3.49	1.42	1.36
3	C	379	IMN	C2-C3	3.49	1.43	1.37
3	D	476	IMN	C12-C11	3.47	1.45	1.38
3	A	379	IMN	C8-N	3.45	1.42	1.36
3	C	379	IMN	C15-C14	3.40	1.44	1.38
3	B	381	IMN	C2-C3	3.38	1.43	1.37
3	D	476	IMN	C8-N	3.29	1.42	1.36
3	C	379	IMN	C15-C10	3.22	1.44	1.39
3	A	379	IMN	C2-C3	3.21	1.42	1.37
3	A	379	IMN	C5-C	3.13	1.47	1.41
3	C	379	IMN	C5-C4	3.09	1.43	1.36
3	C	379	IMN	C8-N	3.02	1.41	1.36
3	A	379	IMN	C5-C4	2.97	1.42	1.36
3	C	379	IMN	C5-C	2.96	1.47	1.41
3	B	381	IMN	C5-C	2.95	1.46	1.41
3	D	476	IMN	C5-C	2.73	1.46	1.41
3	D	476	IMN	C12-C13	2.64	1.43	1.38
3	B	381	IMN	C5-C4	2.63	1.42	1.36
3	A	379	IMN	C12-C13	2.59	1.42	1.38
3	D	476	IMN	C5-C4	2.59	1.42	1.36
3	C	379	IMN	C12-C13	2.51	1.42	1.38
3	A	379	IMN	C4-C3	2.46	1.43	1.38
3	B	381	IMN	C12-C13	2.44	1.42	1.38
3	B	381	IMN	C14-C13	2.34	1.42	1.38
3	C	379	IMN	C4-C3	2.33	1.43	1.38
3	A	379	IMN	C14-C13	2.31	1.42	1.38
3	A	379	IMN	C2-C1	2.23	1.46	1.42
3	D	476	IMN	C14-C13	2.23	1.42	1.38
3	C	379	IMN	C2-C1	2.18	1.46	1.42
3	A	379	IMN	C13-CL	-2.04	1.70	1.74

All (48) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	379	IMN	C17-C7-C8	10.36	135.54	126.41
3	B	381	IMN	C17-C7-C8	9.99	135.22	126.41
3	A	379	IMN	C17-C7-C8	9.95	135.18	126.41
3	D	476	IMN	C17-C7-C8	9.85	135.10	126.41
3	D	476	IMN	C10-C9-N	8.91	128.35	117.95
3	A	379	IMN	C10-C9-N	8.90	128.34	117.95
3	B	381	IMN	C10-C9-N	8.86	128.30	117.95
3	C	379	IMN	C10-C9-N	8.86	128.30	117.95
3	B	381	IMN	C16-C8-N	5.93	129.84	122.37
3	D	476	IMN	C16-C8-N	5.77	129.65	122.37
3	A	379	IMN	C16-C8-N	5.74	129.60	122.37
3	C	379	IMN	C16-C8-N	5.53	129.34	122.37
3	C	379	IMN	C18-C17-C7	4.51	124.74	115.96
3	A	379	IMN	C18-C17-C7	4.22	124.16	115.96
3	B	381	IMN	C18-C17-C7	4.20	124.13	115.96
3	D	476	IMN	C18-C17-C7	4.10	123.94	115.96
3	D	476	IMN	C6-O-C3	4.03	126.27	117.51
3	C	379	IMN	C5-C-C1	-3.97	115.54	120.94
3	A	379	IMN	C5-C-C1	-3.95	115.57	120.94
3	B	381	IMN	C5-C-C1	-3.89	115.65	120.94
3	A	379	IMN	O1-C9-C10	-3.88	112.67	120.23
3	D	476	IMN	O1-C9-C10	-3.86	112.71	120.23
3	D	476	IMN	C5-C-C1	-3.82	115.74	120.94
3	C	379	IMN	O1-C9-C10	-3.82	112.79	120.23
3	B	381	IMN	C6-O-C3	3.80	125.75	117.51
3	D	476	IMN	C15-C10-C9	3.79	128.44	120.26
3	A	379	IMN	C6-O-C3	3.77	125.69	117.51
3	A	379	IMN	C15-C10-C9	3.77	128.39	120.26
3	B	381	IMN	C15-C10-C9	3.74	128.33	120.26
3	C	379	IMN	C15-C10-C9	3.73	128.32	120.26
3	B	381	IMN	O1-C9-C10	-3.73	112.96	120.23
3	C	379	IMN	C6-O-C3	3.70	125.55	117.51
3	D	476	IMN	C11-C10-C9	-2.68	114.47	120.26
3	D	476	IMN	C16-C8-C7	-2.65	123.51	129.24
3	B	381	IMN	C16-C8-C7	-2.65	123.51	129.24
3	A	379	IMN	C11-C10-C9	-2.63	114.59	120.26
3	A	379	IMN	C16-C8-C7	-2.63	123.56	129.24
3	B	381	IMN	C11-C10-C9	-2.56	114.75	120.26
3	C	379	IMN	C11-C10-C9	-2.54	114.78	120.26
3	C	379	IMN	C16-C8-C7	-2.48	123.88	129.24
3	A	379	IMN	O-C3-C2	-2.39	117.91	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	379	IMN	O-C3-C2	-2.27	118.25	124.43
3	B	381	IMN	O-C3-C2	-2.25	118.30	124.43
3	D	476	IMN	O-C3-C2	-2.18	118.49	124.43
3	D	476	IMN	C4-C5-C	2.11	122.94	119.70
3	C	379	IMN	C4-C5-C	2.04	122.83	119.70
3	A	379	IMN	C4-C5-C	2.03	122.81	119.70
3	B	381	IMN	C4-C5-C	2.02	122.80	119.70

There are no chirality outliers.

There are no torsion outliers.

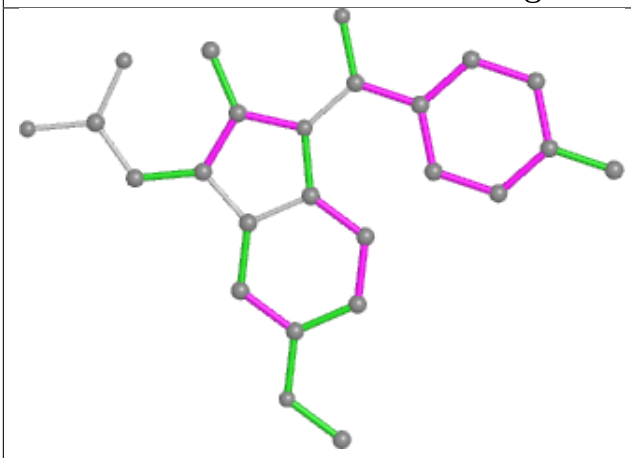
There are no ring outliers.

4 monomers are involved in 8 short contacts:

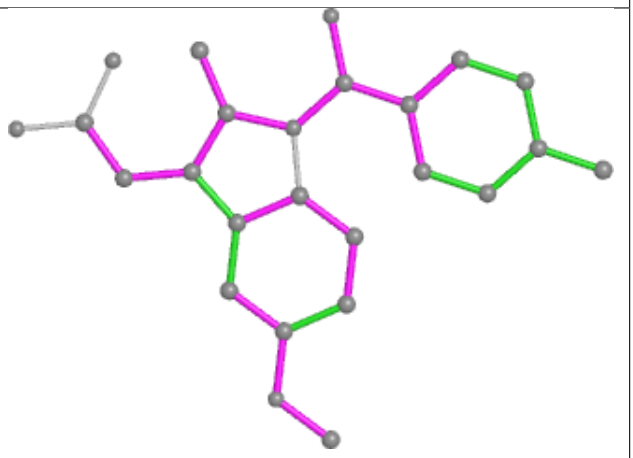
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	381	IMN	2	0
3	A	379	IMN	2	0
3	C	379	IMN	2	0
3	D	476	IMN	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

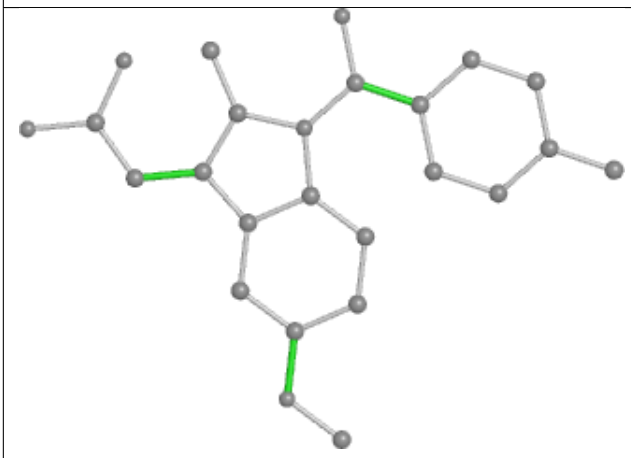
Ligand IMN B 381



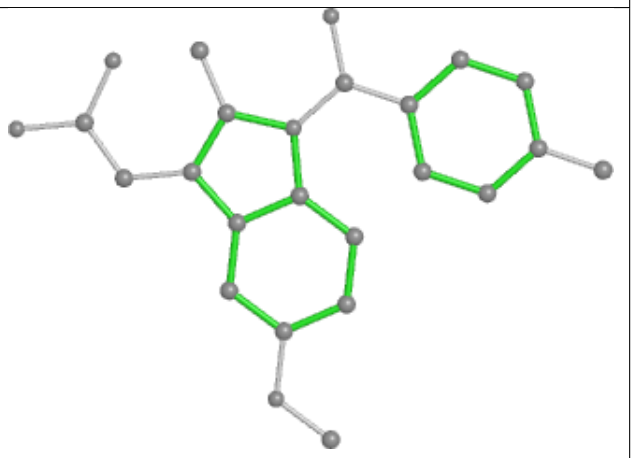
Bond lengths



Bond angles

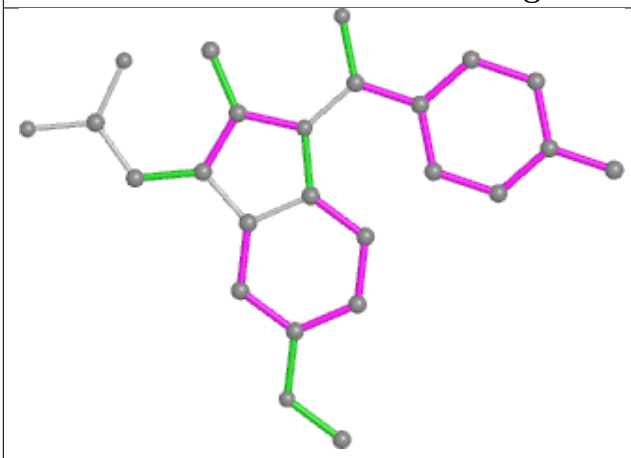


Torsions

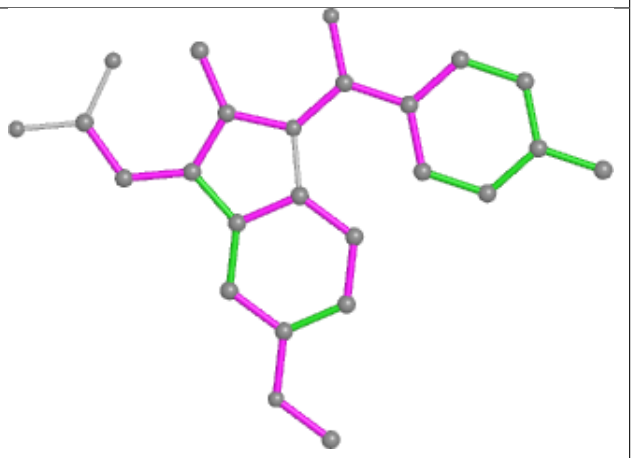


Rings

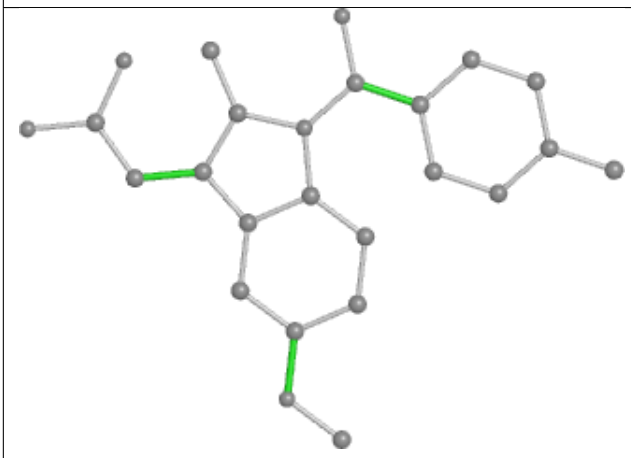
Ligand IMN A 379



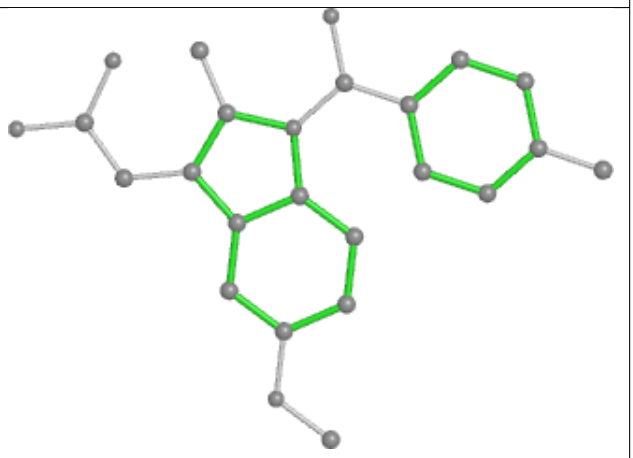
Bond lengths



Bond angles

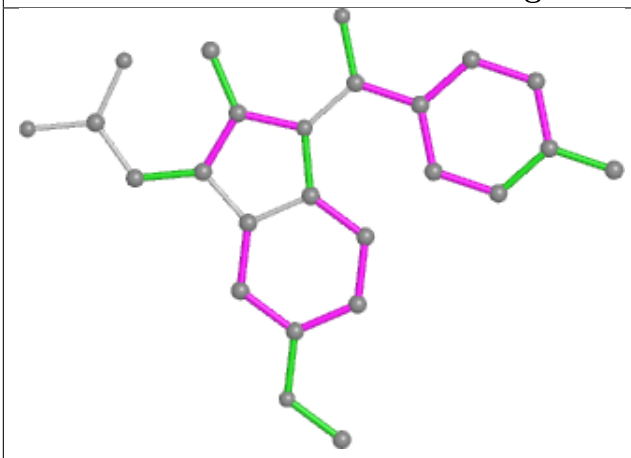


Torsions

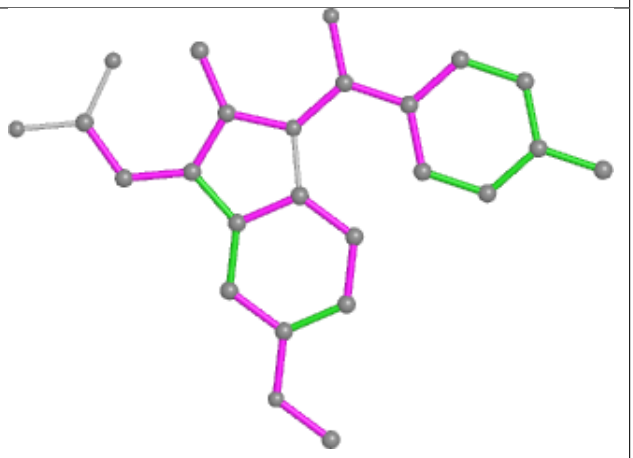


Rings

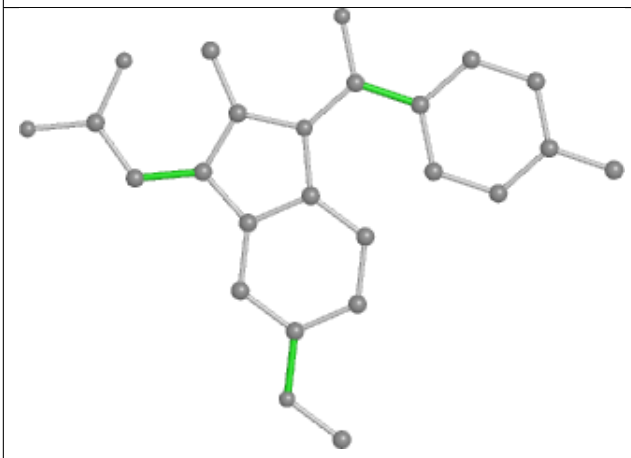
Ligand IMN C 379



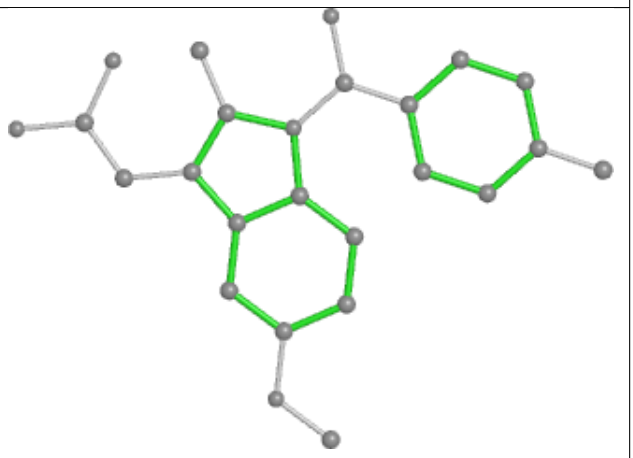
Bond lengths



Bond angles

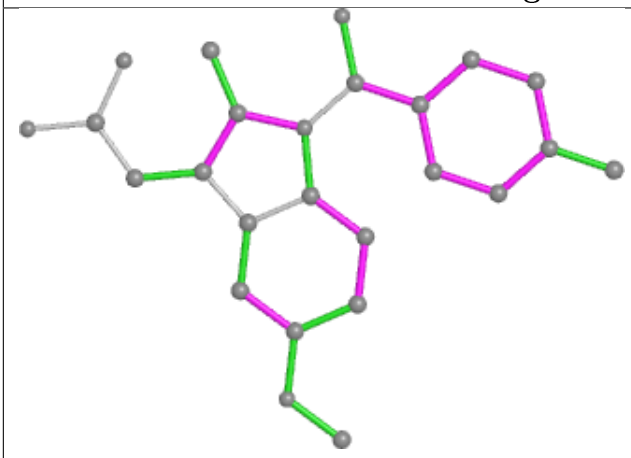


Torsions

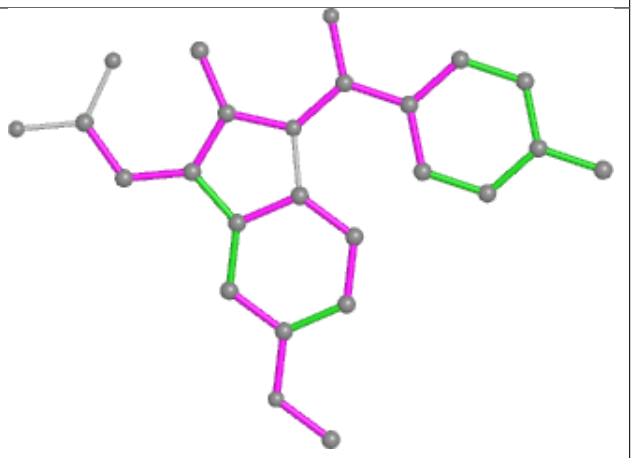


Rings

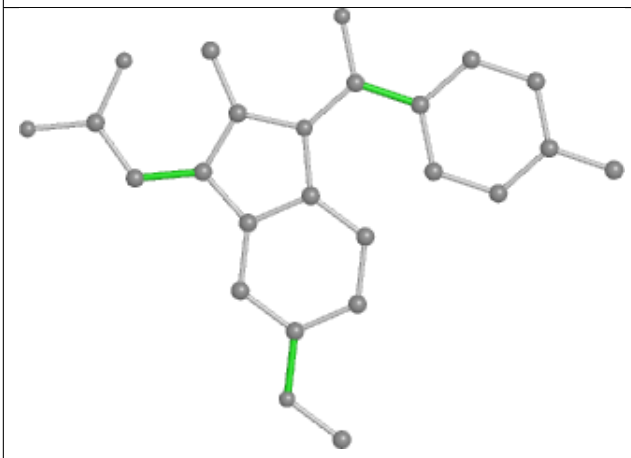
Ligand IMN D 476



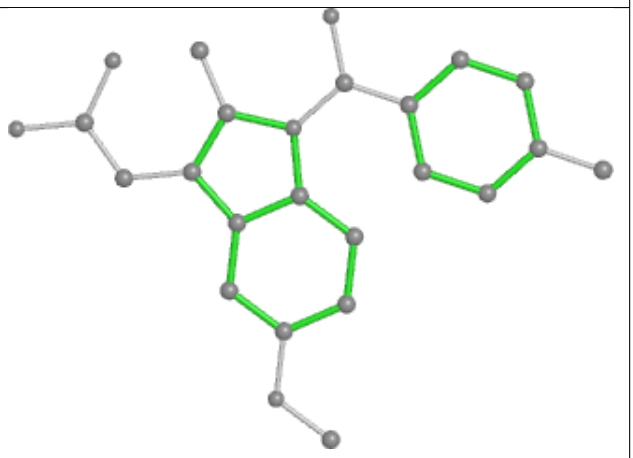
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	274/290 (94%)	-0.91	0	100	100	4, 15, 45, 79	0
1	B	274/290 (94%)	-0.89	0	100	100	3, 14, 49, 66	0
1	C	274/290 (94%)	-0.89	0	100	100	4, 17, 47, 71	0
1	D	274/290 (94%)	-0.85	0	100	100	3, 18, 52, 68	0
All	All	1096/1160 (94%)	-0.89	0	100	100	3, 16, 50, 79	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ACT	B	379	4/4	0.82	0.24	27,30,31,32	0
2	ACT	D	477	4/4	0.85	0.20	10,12,16,18	0
3	IMN	B	381	25/25	0.86	0.17	10,13,20,20	0
3	IMN	D	476	25/25	0.86	0.18	10,13,16,17	0

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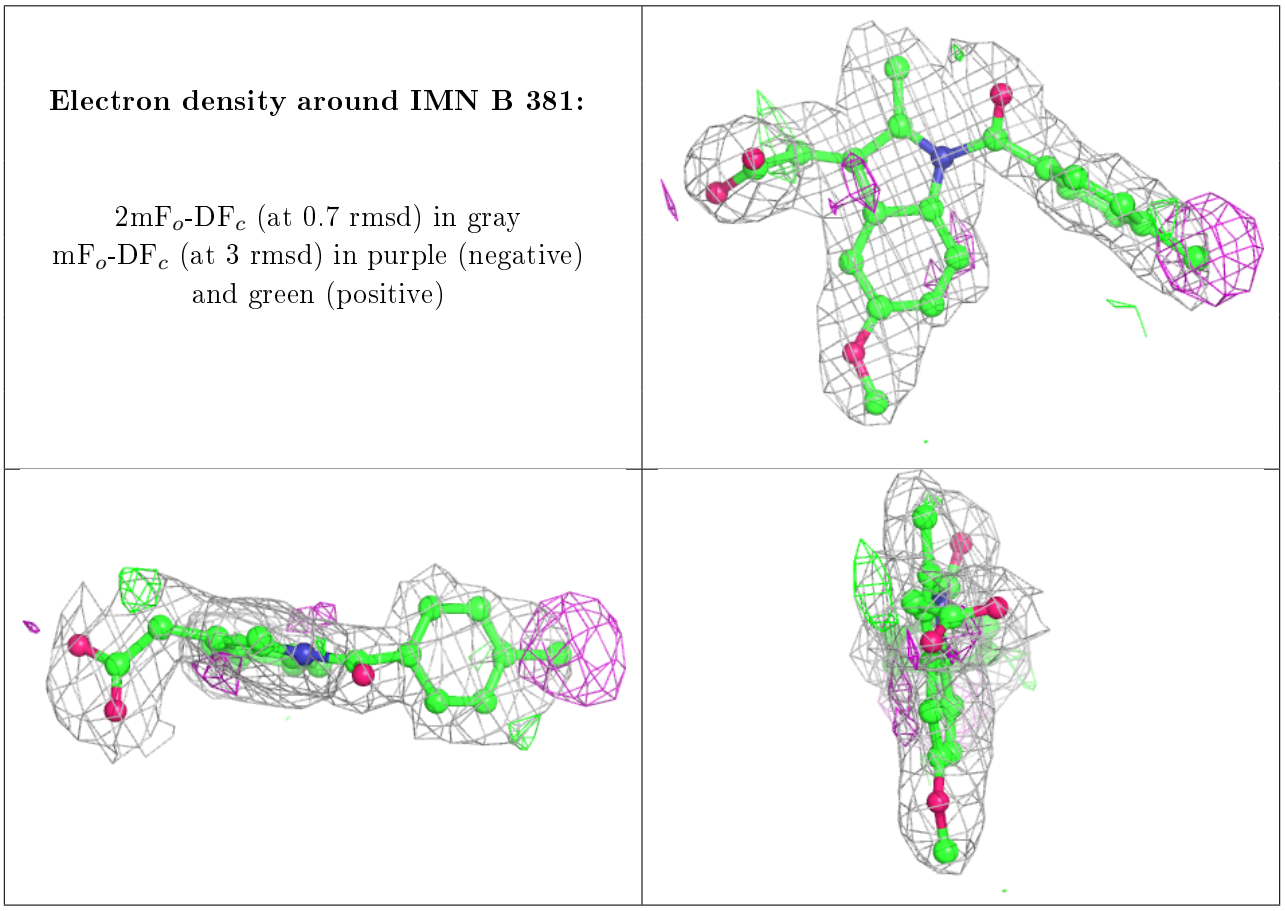
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	IMN	A	379	25/25	0.89	0.15	5,11,17,22	0
3	IMN	C	379	25/25	0.90	0.14	7,9,17,19	0
2	ACT	C	378	4/4	0.92	0.18	13,14,14,16	0
2	ACT	A	378	4/4	0.94	0.14	6,8,10,11	0
4	CL	D	378	1/1	0.95	0.06	13,13,13,13	0
4	CL	D	475	1/1	0.98	0.12	15,15,15,15	0
4	CL	B	380	1/1	0.99	0.07	10,10,10,10	0
4	CL	B	378	1/1	0.99	0.13	15,15,15,15	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

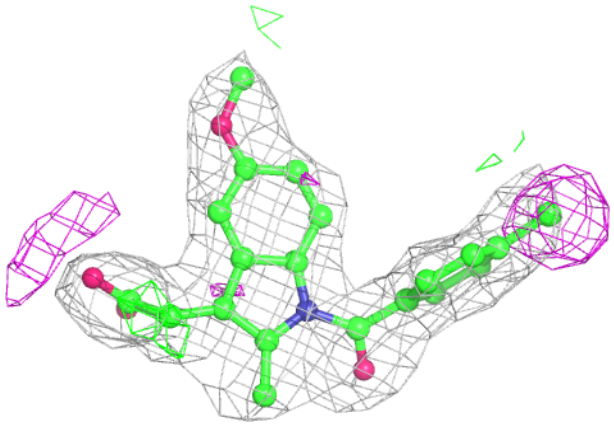
Electron density around IMN B 381:

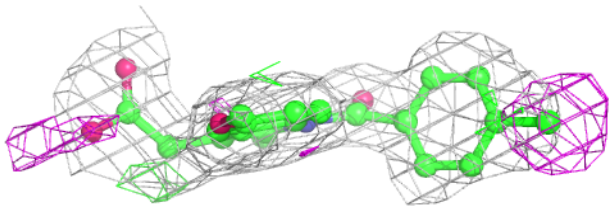
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

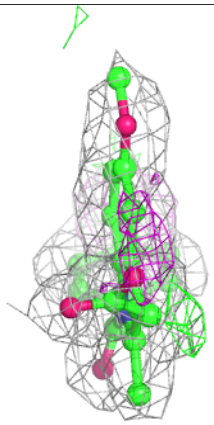


Electron density around IMN D 476:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

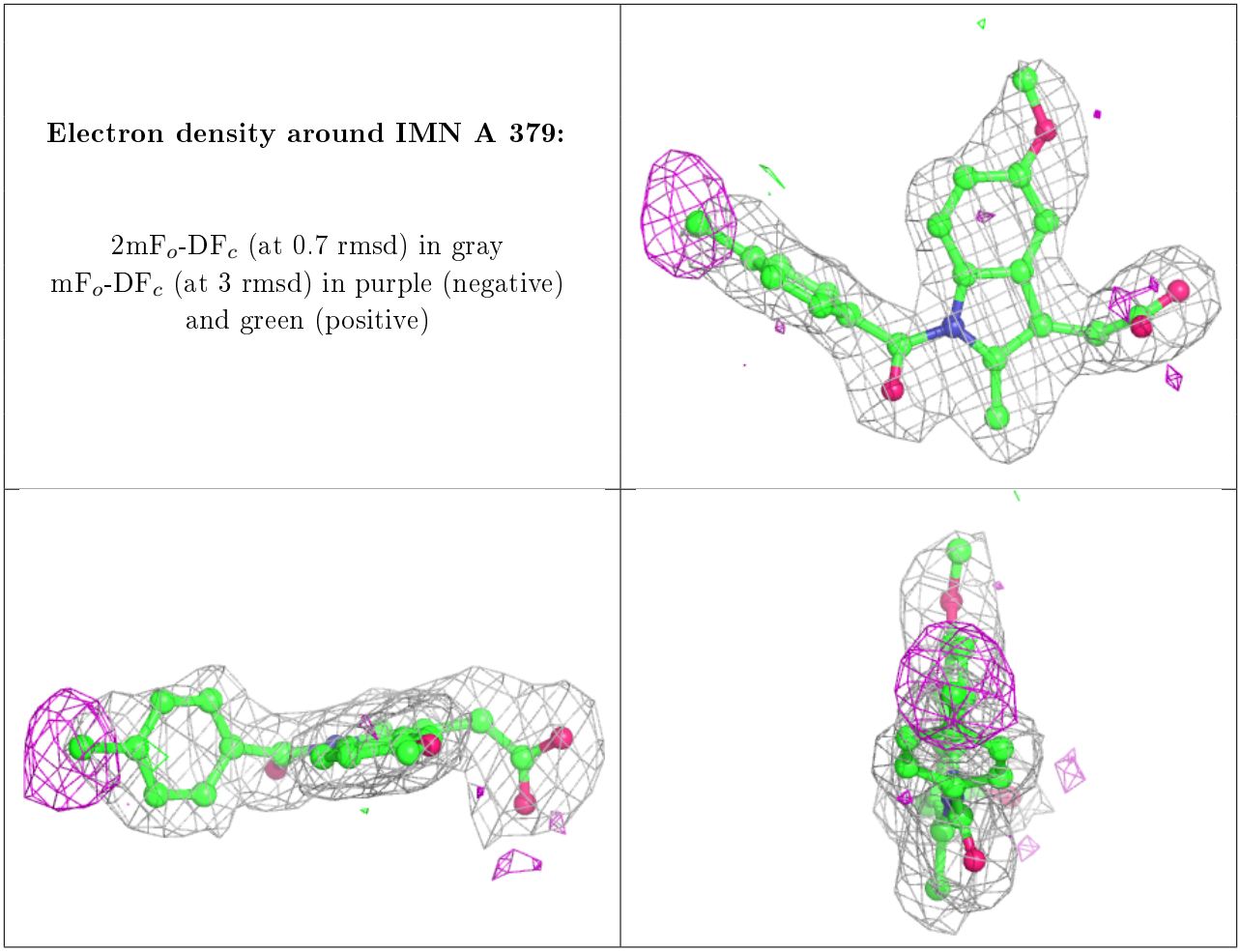






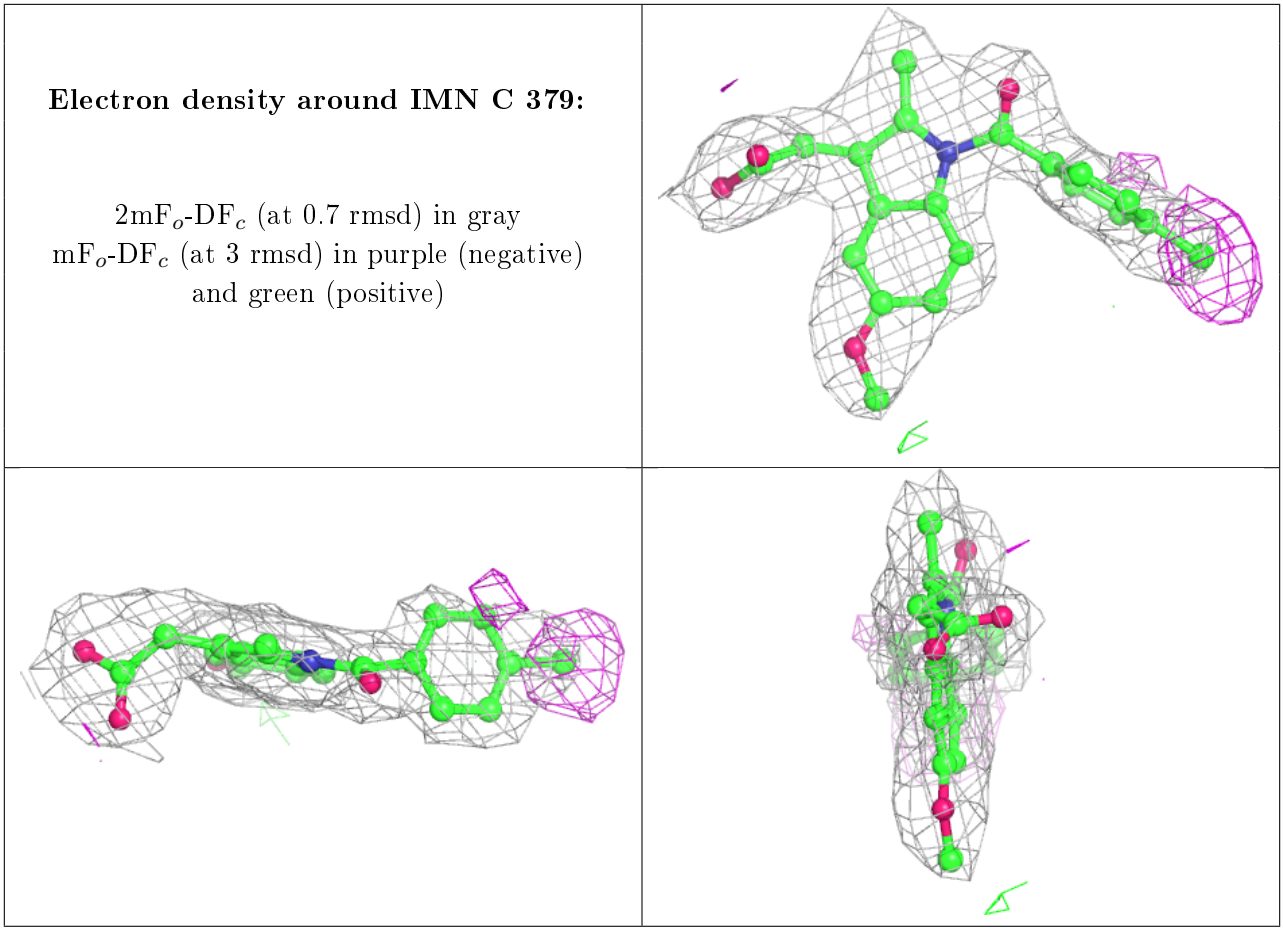
Electron density around IMN A 379:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around IMN C 379:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.